

DETECTING BINOMIALITY

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ABSTRACT. Binomial ideals are special polynomial ideals with many algorithmically and theoretically nice properties. We discuss the problem of deciding if a given polynomial ideal is binomial. While the methods are general, our main motivation and source of examples is the simplification of steady state equations of chemical reaction networks. For homogeneous ideals we give an efficient, Gröbner-free algorithm for binomiality detection, based on linear algebra only. On inhomogeneous input the algorithm can only give a sufficient condition for binomiality. As a remedy we construct a heuristic toolbox that can lead to simplifications even if the given ideal is not binomial.

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1. INTRODUCTION

Non-linear algebra is a mainstay in modern applied mathematics and across the sciences. Very often non-linearity comes in the form of polynomial equations which are much more flexible than linear equations in modeling complex phenomena. The price to be paid is that their mathematical theory—commutative algebra and algebraic geometry—is much more involved than linear algebra. Fortunately, polynomial systems in applications often have special structures. In this paper we focus on *sparsity*, that is, polynomials having few terms.

The sparsest polynomials are monomials. Systems of monomial equations are a big topic in algebraic combinatorics, but in the view of modeling they are not much help.

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Their solution sets are unions of coordinate hyperplanes. The next and more interesting class are *binomial systems* in which each polynomial is allowed to have two terms. Binomials are flexible enough to model many interesting phenomena, but sparse enough to allow a specialized theory [8]. The strongest classical results about binomial systems require one to seek solutions in algebraically closed field such as the complex numbers. However, for the objects in applications (think of concentrations or probabilities) this assumption is prohibitive. One often works with non-negative real numbers and this leads to the fields of real and semi-algebraic geometry. New theory in combinatorial commutative algebra shows that for binomial equations field assumptions can be skirted and that the dependence of binomial systems on their coefficients is quite weak [14]. For binomial equations one can hope for results that do not depend on the explicit values of the parameters and are thus robust in the presence of uncertainty.

The main theme of this paper is how to detect binomiality, that is, how to decide if a given polynomial system is equivalent to a binomial system. The common way to decide binomiality is to compute a Gröbner basis since an ideal can be generated by binomials if and only if any reduced Gröbner basis is binomial [8, Corollary 1.2]. For polynomial systems arising in applications, however, computing a reduced Gröbner basis is often too demanding: as parameter values are unknown, computations have to be performed over the field of rational functions in the parameters. Even though this is computationally feasible, it is time consuming and usually yields an output that is hard to digest for humans. This added complexity comes from the fact that Gröbner bases contain a lot more information than what may be needed for a specific task such as deciding binomiality of a polynomial system. Hence Gröbner-free methods are desirable.

Gröbner-free methods. Gröbner bases started as a generalization of Gauss elimination to polynomials. They have since come back to their roots in linear algebra by the advent of F4 and F5 type algorithms which try to arrange computations so that sparse linear algebra can be exploited [7]. Our method draws on linear algebra in bases of monomials too, and is inspired by these developments in computer algebra.

Deciding if a set of polynomials can be brought into binomial form using linear algebra is the question whether the coefficient matrix has a *partitioning kernel basis* (Definition 2.1 and Proposition 2.5). Deciding this property requires only row reductions and hence is computationally cheap compared to Gröbner bases. It was shown in [18] that, if the coefficient matrix of a suitably extended polynomial system admits a partitioning kernel basis, then the polynomial system is generated by binomials. As a first insight we show that the converse of this need not hold (Example 2.8).

In general computer algebra profits from homogeneity. This is true for Gröbner bases where, for example, Hilbert function driven algorithms can be used to convert a basis for a term-order that is cheap to compute into one for an expensive order, such as lex. We also observe this phenomenon in our Gröbner-free approach: a satisfying answer

to the binomial detection problem can be found if the given system of polynomials is homogeneous. In Section 3 we discuss this case which eventually leads to Algorithm 3.3.

In the inhomogeneous case things are more complicated. Gröbner basis computations can be reduced to the homogeneous case by an easy trick. Detection of binomiality can not (Example 4.1). We address this problem by collecting heuristic approaches that, in the best case, establish binomiality without Gröbner bases (Recipe 4.5). Our approaches can also be used if the system is not entirely binomial, but has some binomials. In Example 4.4 we demonstrate this on a polynomial system from [5].

Binomial steady state ideals. While binomiality detection can be applied to any polynomial system, our motivation comes from chemical reaction network theory where ordinary differential equations with polynomial right-hand sides are used to model dynamic processes in systems biology. The mathematics of these systems is extremely challenging, in particular since realistic models are huge and involve uncertain parameters. As a consequence of the latter, studying dynamical systems arising in biological applications often amounts to studying parameterized families of polynomial ODEs. The first order of business (and concern of a large part of the work in the area) is to determine steady states which are thus the non-negative real zeros of families of parameterized polynomial equations. Moreover, the structure of the polynomial ODEs entails the existence of affine linear subspaces that are invariant for solutions. Hence questions concerning existence and uniqueness of steady states or existence of multiple steady states are equivalent to questions regarding the intersection of the zero set of a parameterized family of polynomials with a family of affine linear subspaces.

If the polynomial equations describing steady states are equivalent to binomial equations (that is, generate a binomial ideal), then their mathematical analysis becomes much easier. This is the main theme of [18]. If a system is binomial, then, for instance, one can decide efficiently if positive steady states exist. If so, then a monomial parametrization can be found using only linear algebra over the integers [8, Section 2], and the steady states are *toric*: they are the positive real part of a toric variety. A sufficient criterion for toric steady states appears in [13, Theorem 4.1]. Since zero sets of general polynomial systems need not have parametrizations at all, we view the task of detecting binomiality as an important step in analyzing polynomials—in systems biology, or other areas like algebraic statistics, control theory, economics, etc.

A frequent and challenging problem in the analysis of dynamical systems in biology is to decide *multistationarity*, that is, the existence of parameter values leading to more than one isolated steady state. A variety of results for precluding multistationarity has appeared in recent years. See, for instance, [12, 21, 3, 1] for methods employing the Jacobian. Similarly, several sufficient criteria for multistationarity have emerged (for example [4, 5]). In general this problem remains very hard. However, in the case of binomial steady state equations, the question of multistationarity can often be answered

effectively, for example positively by [18, Theorem 5.5], or negatively by [17, Theorem 1.4]. Both of these results require only the study of systems of linear inequalities.

Notation. In this paper we work with the polynomial ring $\mathbb{k}[x_1, \dots, x_n]$ in n variables. The coefficient field \mathbb{k} is usually \mathbb{R} , or the field of real rational functions in a set of parameters. Our methods are agnostic towards the field. A system of polynomial equations $f_1 = f_2 = \dots = f_s = 0$ in the variables x_1, \dots, x_n is encoded in the *ideal* $\langle f_1, \dots, f_s \rangle \subset \mathbb{k}[x_1, \dots, x_n]$. A polynomial is *homogeneous* if all its terms have the same total degree, and an ideal is homogeneous if it can be generated by homogeneous polynomials. A *binomial* is a polynomial with at most two terms. In particular, a monomial is a binomial. It is important to distinguish between binomial ideals and binomial systems. A *binomial system* $f_1 = \dots = f_s = 0$ is a polynomial system such that each f_i is a binomial. In contrast, an ideal $\langle f_1, \dots, f_s \rangle$ is a *binomial ideal* if there exist binomials that generate the same ideal. Thus general non-binomials do not form a binomial system, even if they generate a binomial ideal. For the sake of brevity we will not give an introduction to commutative algebra here, but refer to standard text books like [6, 2]. The very modest amount of matroid theory necessary in Section 2 can be picked up from the first pages of [20].

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2. GRÖBNER-FREE CRITERIA FOR BINOMIALITY

The most basic criterion to decide if an ideal is binomial is to compute a Gröbner basis. This works because the Buchberger algorithm is binomial-friendly: an S-pair of binomials is a binomial. Since the reduced Gröbner basis is unique and must be computable from the binomial generators, it consists of binomials if and only if the ideal is binomial. However, Gröbner bases can be very hard to compute, so other criteria using only linear algebra are also desirable. Linear algebra enters, when we write a polynomial system as $A\Psi(x)$, the product of a coefficient matrix A with entries in \mathbb{k} , and a vector of monomials $\Psi(x)$. Clearly, if we use row operations on the matrix to bring it into a form where each row has at most two non-zero entries, then the ideal is generated by binomials and monomials. This criterion is too naive to detect all binomial ideals since it allows only \mathbb{k} -linear combinations of the given polynomials. We show in Section 3 that, at least for homogeneous ideals, it can be extended to a characterization. Before we embark into the details, we formalize the condition on the matrix.

Definition 2.1. A matrix A has a *partitioning kernel basis* if its kernel admits a basis of vectors with disjoint supports, that is, if there exists a basis $b^{(1)}, \dots, b^{(d)}$ of $\ker(A)$ such that $\text{supp}(b^{(i)}) \cap \text{supp}(b^{(j)}) = \emptyset$ for all $i \neq j$.

The following proposition allows one to check for a partitioning kernel basis with linear algebra. The underlying reason is the very restricted structure of the kernel, expressed best in matroid language.

Proposition 2.2. *The following are equivalent for any matrix A .*

- 1) *A has a partitioning kernel basis.*
- 2) *The column matroid of A is a direct sum of uniform matroids $U_{r-1,r}$ of corank one, and possibly several coloops $U_{1,1}$.*
- 3) *The reduced row echelon form of A has at most two non-zero entries in each row.*

Proof. **1 \Rightarrow 2:** Let b_1, \dots, b_k be the partitioning kernel basis. The supports of this basis satisfy the circuit axioms and are thus equal to the circuits of the column matroid of A . Indeed, non-containment and circuit elimination are satisfied trivially because there is no overlap between any two circuits. For any non-zero element $\tilde{b} \in \ker(A)$, we have $\tilde{b} = \sum_i \lambda_i b_i$. By the partitioning kernel basis property $\text{supp}(\tilde{b}) = \bigcup_i \{\text{supp}(b_i) : \lambda_i \neq 0\}$, so either \tilde{b} is proportional to one of the b_i , or its support properly contains the support of a circuit, so it cannot be a circuit. The columns of A which do not appear in any circuit are coloops and the remaining columns form a direct sum of k uniform matroids of corank one.

2 \Rightarrow 3: If the column matroid of A is a direct sum of matroids, then the unique reduced row echelon form has block structure corresponding to the direct sum decomposition. Therefore it suffices to consider a single block which has one-dimensional kernel of full support (the coloops are (1×1) -identity blocks). Ignoring zero rows, the reduced row echelon form of such a matrix is $(I_{r-1}|c)$ where $r - 1$ is the rank and $c \in \mathbb{k}_{\neq 0}^{r-1}$.

3 \Rightarrow 1: Rows of the reduced row echelon form with exactly one non-zero entry correspond to positions where every element of the kernel has a zero. Thus we can assume that there are none and each row of A has exactly two non-zero entries. Let c be a non-pivotal column with $r - 1$ non-zero entries. The restriction of A to c and the corresponding pivotal columns yields a block containing $(I_{r-1}|c)$ and some zero rows. The unique kernel vector corresponding to the dependencies in this block is orthogonal to the kernel of the remaining columns. This procedure can be applied to any non-pivotal column. The thus constructed basis is a partitioning kernel basis. \square

Remark 2.3. Proposition 2.2 shows that the complexity of deciding if a matrix has a partitioning kernel basis is essentially the same as that of Gauss-Jordan elimination. One needs $O(n^3)$ field operations where n is the larger of the dimensions of the matrix.

Remark 2.4. A direct sum of (arbitrary) uniform matroids is called a partition matroid.

We now translate Proposition 2.2 to polynomial systems.

Proposition 2.5. *If A has a partitioning kernel basis, and $\Psi(x)$ is a vector of monomials of appropriate length, then the ideal $\langle A\Psi(x) \rangle \subset \mathbb{k}[x_1, \dots, x_n]$ is binomial. If*

$A\Psi(x)$ is any system that can be transformed into a binomial system using only \mathbb{k} -linear combinations, then A has a partitioning kernel basis.

Proof. Up to coloops the first part is [18, Theorem 3.3] and the coloops only give monomials. The second statement is clear since \mathbb{k} -linear combinations of polynomials are row operations on the coefficient matrix and those do not change the kernel. \square

Our general strategy is to suitably extend a given system $A\Psi(x)$ with redundant polynomials such that Proposition 2.5 yields binomiality of an extended system $A'\Psi'(x)$. This happens in the following example.

Example 2.6. Let $f_1 = x - y$, $f_2 = z - w$, and $f_3 = x(f_1 + f_2) = x^2 - xy + xz - xw$. Ordering the monomials $\Psi^T = (x, y, z, w, x^2, xy, xz, xw)$, the system linearizes as

$$f = (f_1, f_2, f_3) = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix} \cdot \Psi.$$

The coefficient matrix is in reduced row echelon form and does not have a partitioning kernel basis by Proposition 2.2. Algorithm 3.3 takes this problem into account, working degree by degree. The ideal is binomial since f_3 is a binomial (in fact, zero) in the quotient ring $\mathbb{k}[x, y, z]/\langle x - y, z - w \rangle$.

The first hint into how to extend A and $\Psi(x)$ is the following theorem due to Pérez Millán et al.

Theorem 2.7 ([18, Theorem 3.19]). *Let $f_1 = f_2 = \dots = f_s = 0$ be a polynomial system. If there exist monomials $x^{\alpha_1}, \dots, x^{\alpha_m}$ such that, for some $i_1, \dots, i_m \in [s]$, the system*

$$(2.1) \quad f_1 = f_2 = \dots = f_s = x^{\alpha_1} f_{i_1} = \dots = x^{\alpha_m} f_{i_m} = 0$$

has a coefficient matrix with a partitioning kernel basis, then $\langle f_1, \dots, f_s \rangle$ is binomial.

Theorem 2.7 is true since the additional generators in (2.1) do not change the ideal that the system generates. This together with the explicit description of the binomial generators in the case of a partitioning kernel basis [18, Theorem 3.3] yields the result. If the condition in Theorem 2.7 were also necessary, then a test for binomiality could be built on trying to systematically identify the monomials x^α . However, the converse of Theorem 2.7 is not true.

Example 2.8. Let $I = \langle f_1, f_2 \rangle$ be the homogeneous binomial ideal generated by the non-binomials $f_1 = x - y + x^2 + y^2 + z^2$, $f_2 = x^2 + y^2 + z^2$. For no choice of monomials $m_{11}, \dots, m_{1r}, m_{21}, \dots, m_{2s} \in \mathbb{k}[x, y, z]$ does the coefficient matrix of the system

$$(2.2) \quad f_1 = m_{11}f_1 = \dots = m_{1r}f_1 = f_2 = m_{21}f_2 = \dots = m_{2s}f_2 = 0$$

have a partitioning kernel basis.

For the proof Example 2.8 we first need the following curious little fact.

Lemma 2.9. *The ideal $I = \langle x^2 + y^2 + z^2 \rangle \subset \mathbb{k}[x, y, z]$ does not contain a non-zero binomial.*

Proof. We can assume that \mathbb{k} is algebraically closed, since if I contains a non-zero binomial, then so does its extension to the algebraic closure. Assume that for some $f \in \mathbb{k}[x, y, z]$, the product $b = f(x^2 + y^2 + z^2) \in I$ is a binomial. We can assume that b is not divisible by any variable. Indeed, if a variable divides b , then it divides f and we find a lower degree binomial in I . Since I is homogeneous, we can also assume that b is homogeneous. Potentially renaming the variables, we can assume $b = x^d - \lambda y^s z^{d-s}$ for some $0 \leq s < d$ and $\lambda \in \mathbb{k}$. Since \mathbb{k} is algebraically closed, there is a solution ξ to the equation $x^2 = -1$. The generator $x^2 + y^2 + z^2$ vanishes at $(\xi, 1, 0)$ but b does not vanish there. This contradiction shows that I cannot contain a binomial. \square

Proof of Example 2.8. Let d be the highest total degree among monomials in the system (2.2) and consider the restriction of all involved polynomials to degree d . Since the highest degree part of both f_1 and f_2 equals $(x^2 + y^2 + z^2)$, only monomial multiples of $(x^2 + y^2 + z^2)$ can contribute to the degree d part of the system (2.2). If the whole coefficient matrix of (2.2) had a partitioning kernel basis, then also the submatrix with only the columns for degree d monomials had one (Proposition 2.2). In this case row reductions on the submatrix would yield a binomial in degree d in the ideal generated by $(x^2 + y^2 + z^2)$. This is impossible by Lemma 2.9. \square

Example 2.8 may seem contrived, but this kind of “trivial obfuscation” of binomials does happen in applications. Of course, for humans it is obvious that one should first isolate the linear binomial $x - y$ and then search for implied quadratic binomials which reduce the trinomial. Our next aim is Algorithm 3.3 which implements this idea, at least in the homogeneous case. The homogeneity assumption cannot be skirted, unfortunately. It is true that an ideal is binomial if and only if its homogenization is binomial [8, Corollary 1.4], but the homogenization is not accessible without a Gröbner basis. It would be superb for our purposes if homogenizing the generators of a binomial ideal would always yield a binomial ideal. Unfortunately this is not the case as Example 4.1 shows.

3. THE HOMOGENEOUS CASE

If a given ideal I is homogeneous, the graded vector space structure of the quotient $\mathbb{k}[x_1, \dots, x_n]/I$ allows one to check binomiality degree by degree. For this we need some basic facts about quotients modulo binomials (see [8, Section 1] for details). Any set of binomials B in $\mathbb{k}[x_1, \dots, x_n]$ induces an equivalence relation on the set of monomials in $\mathbb{k}[x_1, \dots, x_n]$ under which $m_1 \sim m_2$ if and only if $m_1 - \lambda m_2 \in \langle B \rangle$ for some non-zero $\lambda \in \mathbb{k}$. As a \mathbb{k} -vector space the quotient ring $\mathbb{k}[x_1, \dots, x_n]/\langle B \rangle$ is spanned by the equivalence classes of monomials and those are all linearly independent [8, Proposition 1.11]. If the binomials are homogeneous, then the situation is particularly nice. For example, the

equivalence classes are finite and elements of the quotient have well-defined degrees. The notions of monomial, binomial, and polynomial are extended to the quotient ring. For example, a binomial is a polynomial that uses at most two equivalence classes of monomials. The unified mathematical framework to treat quotients modulo binomials are monoid algebras, but we refrain from introducing this notion here.

As a consequence of the discussion above, a polynomial system $f_1 = \dots = f_s = 0$ can be considered modulo binomials, and the coefficient matrix of the quotient system is well-defined. It arises from the coefficient matrix of the original system by summing columns for monomials in the same equivalence class.

Example 3.1. In $\mathbb{k}[x, y]$, let $b = x^2 - y^2$. Among monomials of total degree three, x^3 and xy^2 , as well as x^2y and y^3 become equal in $\mathbb{k}[x, y]/\langle b \rangle$. Thus the degree three part in the quotient is two-dimensional with one basis vector per equivalence class. Consequently, the trinomial $f = x^3 + xy^2 + y^3$ maps to a binomial with coefficient matrix $[2, 1]$. This matrix arises from the matrix $[1, 1, 1, 0]$ by summing the columns corresponding to x^3 and xy^2 , as well as those for x^2y and y^3 .

The reduction modulo lower degree binomials in Example 3.1 can be done in general.

Lemma 3.2. *Let $f_1, \dots, f_s \in \mathbb{k}[x_1, \dots, x_n]$ be homogeneous polynomials of degree d , and $B \subset \mathbb{k}[x_1, \dots, x_n]$ a set of homogeneous binomials of degree at most d . Then in the quotient ring $\mathbb{k}[x_1, \dots, x_n]/\langle B \rangle$ the ideal $\langle f_1, \dots, f_s \rangle/\langle B \rangle$ is binomial if and only if the coefficient matrix of the images of f_1, \dots, f_s in $\mathbb{k}[x_1, \dots, x_n]/\langle B \rangle$ has a partitioning kernel basis.*

Proof. The graded version of Nakayama's lemma (see Corollary 4.8b together with Exercise 4.6 in [9]) implies that the ideal $\langle f_1, \dots, f_s \rangle/\langle B \rangle \subset \mathbb{k}[x_1, \dots, x_n]/\langle B \rangle$ has a well-defined number of minimal generators in each degree. Therefore any minimal generating set consists only of degree d polynomials and Proposition 2.5 applied to the finite-dimensional vector space of degree d polynomials correctly decides binomiality. \square

Lemma 3.2 is the basis for the following binomial detection algorithm.

Algorithm 3.3.

Input: Homogeneous polynomials $f_1, \dots, f_s \in \mathbb{k}[x_1, \dots, x_n]$.

Output: Yes and a binomial generating set of $\langle f_1, \dots, f_s \rangle$ if one exists, No otherwise.

1) Let

- $B := \emptyset$,
- $R := \mathbb{k}[x_1, \dots, x_n]$,
- $F := \{f_1, \dots, f_s\}$.

2) While F is not empty,

- a) Let F_{\min} be the set of elements of minimal degree in F .
- b) Redefine $F := F \setminus F_{\min}$.
- c) Compute the reduced row echelon form A of the coefficient matrix of F_{\min} .

- d) If A has a row with three or more non-zero entries, output No and stop.
 - e) Find a set B' of binomials in $\mathbb{k}[x_1, \dots, x_n]$ whose images in R generate $\langle F_{\min} \rangle$ and redefine $B := B \cup B'$.
 - f) Redefine $R := \mathbb{k}[x_1, \dots, x_n]/\langle B \rangle$.
 - g) Redefine F as its image in R .
- 3) Output Yes and B .

Proof of correctness and termination. Termination is obvious. In fact, the maximum number of iterations in the while loop equals the number of distinct total degrees among f_1, \dots, f_s . Step 2.d relies on Proposition 2.2. In step 2.e, binomials that generate $\langle F_{\min} \rangle$ in R can be read off the reduced row echelon form via Proposition 2.2. Then any preimages in $\mathbb{k}[x_1, \dots, x_n]$ of those binomials suffice for B' . Lemma 3.2 shows that the while loop either exhausts F if $\langle f_1, \dots, f_s \rangle$ is binomial, or stops when this is not the case. \square

Remark 3.4. In the homogeneous case there is a natural choice of finite-dimensional vector spaces to work in: polynomials of a fixed degree. In each iteration of the while loop in Algorithm 3.3, the rows of A span the vector space of polynomials of degree d in the ideal (modulo the binomials in $\langle B \rangle$). In the general inhomogeneous situation extra work is needed to construct a suitable finite-dimensional vector space. In particular, one needs to select from the infinite list of binomials in the ideal not too many, but enough to reduce all given polynomials to binomials whenever this is possible. An interesting problem for the future is to adapt one of the selection strategies from the F4 algorithm for Gröbner bases [10] for this task.

Remark 3.5. Coefficient matrices of polynomial systems are typically very sparse. An efficient implementation of Algorithm 3.3 has to take this into account.

Remark 3.6. Algorithm 3.3 could also be written completely in the polynomial ring without any quotients. Then in each new degree, one would have to consider the coefficient matrix of F_{\min} together with all binomials of degree d in the ideal $\langle B \rangle$. This list grows very quickly and so does the list of monomials appearing in these binomials. Thus it is not only more elegant to work with the quotient, but also more efficient.

To implement Algorithm 3.3 completely without Gröbner bases some refinements are necessary. Simply using $R = \mathbb{k}[x_1, \dots, x_n]/B$ in MACAULAY2 will make it compute a Gröbner basis of B to effectively work with the quotient. For our purposes, however, this is not necessary.

Proposition 3.7. *Algorithm 3.3 can be implemented without Gröbner bases.*

Proof. The critical step is 2.g, when the algorithm reduces F modulo the binomials already found. For the following step 2.c elements of F_{\min} need to be written in terms of a basis of the finite-dimensional vector space $R_{\deg(F_{\min})}$ of degree $\deg(F_{\min})$ monomials modulo the binomials in B . The equivalence relation introduced in the beginning of this

section can also be thought of as a graph on monomials, and thus these reductions can be carried out with graph enumeration algorithms like breadth first search. Restricting to monomials of degree $\deg(F_{\min})$, the connected components are a vector space basis of $R_{\deg(F_{\min})}$ and can thus be used to gather coefficients in step 2.g. \square

Remark 3.8. The feasibility of graph-theoretic computations in cases where Gröbner bases cannot be computed has been demonstrated in [15]. Example 4.9 there contains a binomial ideal whose Gröbner basis cannot be computed, but whose non-radicality was proved using a graph-theoretic computation. This yielded a negative answer to the question of radicality of conditional independence ideals in algebraic statistics.

Remark 3.9. Using Gröbner bases one represents each connected component of the graph defined by $\langle B \rangle$ by its least monomial with respect to the term order. Our philosophy is that this is not necessary: one should work with the connected components per se. Why bother with picking and finding a specific representative in each component if any representative works? In an implementation one could choose a data structure that for each monomial stores an index of the connected component it belongs to.

Remark 3.10. It is trivial to generate classes of examples where Gröbner bases methods fail, but Algorithm 3.3 is quick. For example, take any set of binomials whose Gröbner basis cannot be computed and add any polynomial in the ideal. Algorithm 3.3 immediately goes to work on reducing the polynomial modulo the binomials, while any implementation of Gröbner bases embarks into its hopeless task.

Remark 3.11. Remark 3.10 highlights the Gröbner-free spirit of our method. The Gröbner basis of an ideal contains much more information than binomiality. One should avoid expensive computation to decide this simple question.

4. HEURISTICS FOR THE INHOMOGENEOUS CASE

The ideals one encounters in chemical reaction network theory are often not homogeneous, so that the results from Section 3 do not apply. The first idea one may have for the inhomogeneous case is to work with some (partial) homogenization. Gröbner bases are quite robust in relation to homogenization. For example, to compute a Gröbner basis of a non-homogeneous ideal it suffices to homogenize the generators, compute a Gröbner basis of this homogeneous ideal, and then dehomogenize. Although the intermediate homogeneous ideal is generally not equal to the homogenization of the original ideal, the dehomogenized Gröbner basis is a Gröbner basis of the dehomogenized ideal [2, Exercise 1.7.8].

Unfortunately the notion of binomiality does not lend itself to that kind of tricks. Geometrically, homogenizing (all polynomials in) an ideal yields the projective closure and dehomogenizing restricts to one affine piece. Homogenizing only the generators creates extra components *at infinity* and these components need not be binomial. Even

if they are binomial, the intersection need not be binomial (see also [14, Problem 17.1]). This is the case in the following example.

Example 4.1. The ideal $\langle ab - x, ab - y, x + y + 1 \rangle \subset \mathbb{K}[a, b, x, y]$ is binomial as it equals $\langle 2y + 1, 2x + 1, 2ab + 1 \rangle$. Homogenizing the generators, however, yields the non-binomial ideal $\langle ab - xz, ab - yz, x + y + z \rangle$.

We now present some alternatives that do not give complete answers but are quick to check. They can be applied before resorting to an expensive Gröbner basis computation.

The quickest (but least likely to be successful) approach is to try linear algebraic manipulations of the given polynomials. Equivalently one applies row operations to the coefficient matrix, for instance, computing the reduced row echelon form. If it has a partitioning kernel basis, then the ideal is binomial and all non-binomial generators are \mathbb{K} -linear combinations of the binomials. While it may seem very much to ask for this, it does happen for the family of networks in [18, Section 4].

If just linear algebra is not successful, one can homogenize the generators and run Algorithm 3.3. If the resulting homogeneous ideal comes out binomial, then the original ideal was binomial by the following simple fact, proven for instance in [2, Corollary A.4.16].

Proposition 4.2. *Let $I \subset \mathbb{K}[x_1, \dots, x_n]$ be an ideal and $I' \subset \mathbb{K}[x_0, x_1, \dots, x_n]$ the homogeneous ideal generated by the homogenizations of the generators of I (using variable x_0). Then I is generated by the dehomogenization of any generating set of I' .*

We now illustrate a phenomenon leading to failure of the above heuristics.

Example 4.3. Consider the network from [18, Example 3.15]. The steady states are non-negative real zeros of the following polynomials.

$$\begin{aligned} f_1 &= -k_{12}x_1 + k_{21}x_2 - k_{1112}x_1x_7 + (k_{1211} + k_{1213})x_9, \\ f_2 &= k_{12}x_1 - k_{21}x_2 - k_{23}x_2 + k_{32}x_3 + k_{67}x_6, \\ f_3 &= k_{23}x_2 - k_{32}x_3 - k_{34}x_3 - k_{89}x_3x_7 + k_{910}x_8 + k_{98}x_8, \\ f_4 &= k_{34}x_3 - k_{56}x_4x_5 + k_{65}x_6, \\ f_5 &= -k_{56}x_4x_5 + k_{65}x_6 + k_{910}x_8 + k_{1213}x_9, \\ f_6 &= k_{56}x_4x_5 - (k_{65} + k_{67})x_6, \\ f_7 &= k_{67}x_6 - k_{1112}x_1x_7 - k_{89}x_3x_7 + k_{98}x_8 + k_{1211}x_9, \\ f_8 &= k_{89}x_3x_7 - (k_{910} + k_{98})x_8, \\ f_9 &= k_{1112}x_1x_7 - (k_{1211} + k_{1213})x_9. \end{aligned}$$

The binomials f_6 , f_8 , and f_9 can be used to eliminate one of every pair (x_6, x_4x_5) , (x_8, x_3x_7) , and (x_9, x_1x_7) . We eliminate x_4x_5 , x_8 , and x_9 . It can be checked that eliminating x_1x_7 instead of x_9 does not lead to binomials immediately (although it leads to

linear trinomials).

$$\begin{aligned}
f'_1 &= -k_{12}x_1 + k_{21}x_2, \\
f'_2 &= k_{12}x_1 - (k_{21} + k_{23})x_2 + k_{32}x_3 + k_{67}x_6, \\
f'_3 &= k_{23}x_2 - (k_{32} + k_{34})x_3, \\
f'_4 &= k_{34}x_3 - k_{67}x_6, \\
f'_5 &= -k_{67}x_6 + \frac{k_{1112}k_{1213}x_1x_7}{k_{1211} + k_{1213}} + \frac{k_{89}k_{910}x_3x_7}{k_{910} + k_{98}}, \\
f'_7 &= k_{67}x_6 - \frac{(k_{1112}k_{1213}(k_{910} + k_{98})x_1 + (k_{1211} + k_{1213})k_{89}k_{910}x_3)x_7}{(k_{1211} + k_{1213})(k_{910} + k_{98})}.
\end{aligned}$$

Using the linear relations f'_1 and f'_3 the remaining system is recognized to consist of only two independent binomials:

$$\begin{aligned}
f''_2 &= -k_{34}x_3 + k_{67}x_6 \\
f''_4 &= k_{34}x_3 - k_{67}x_6, \\
f''_5 &= -k_{67}x_6 + \left(\frac{k_{1112}k_{1213}k_{21}}{k_{12}(k_{1211} + k_{1213})} + \frac{k_{23}k_{89}k_{910}}{(k_{32} + k_{34})(k_{910} + k_{98})} \right) x_2x_7, \\
f''_7 &= k_{67}x_6 + \left(-\frac{k_{1112}k_{1213}k_{21}}{k_{12}(k_{1211} + k_{1213})} - \frac{k_{23}k_{89}k_{910}}{(k_{32} + k_{34})(k_{910} + k_{98})} \right) x_2x_7.
\end{aligned}$$

This analysis shows that the steady state ideal under consideration equals the binomial ideal $\langle f'_1, f''_2, f'_3, f''_5, f_6, f_8, f_9 \rangle$. The Gröbner basis computation in [18, Example 3.15] also yields the result, but it is arguably less instructive. Note also that naive homogenization does not yield binomiality. The element f_2 is linear. After homogenization, Algorithm 3.3 would pick only this element as F_{\min} and stop since it is not a binomial.

The effect in Example 4.3 motivates our final method: term replacements using known binomials. We expect this to be very useful in applications from system biology for the following reasons.

- It often happens that non-binomial generators are linear combinations of binomials as in Example 4.3 where $f_1 = f'_1 + f_9$.
- Steady state ideals of networks with enzyme-substrate complexes always have some binomial generators. These complexes are produced by only one reaction and thus their rate of change is binomial.
- In MAPK networks, which describe certain types of cellular signaling, one often finds binomials of the form $kx_ax_b - k'x_c$.
- Frequently binomials in steady state ideals are linear. Equivalently some of the concentrations are equal up to a scaling (which may depend on kinetic parameters). This happens for all examples in [19].

We now illustrate term replacements in a larger example which comes from the network for ERK activation embedded in two negative feedback loops (see [5, Section 5] for pointers to the relevant biology).

Example 4.4. Consider the following steady state ideal generated by 29 polynomials.

$$\begin{aligned}
f_1 &= -k_1x_1x_2 + k_2x_3 + k_6x_6, & f_2 &= -k_1x_1x_2 + k_2x_3 + k_3x_3, & f_3 &= k_1x_1x_2 - k_2x_3 - k_3x_3, \\
f_4 &= k_{11}x_{10} + k_{12}x_{10} + k_{38}x_{25} + k_{42}x_{27} + k_3x_3 - k_{37}x_{18}x_4, \\
&\quad - k_4x_4x_5 + k_5x_6 - k_7x_4x_7 + k_8x_8 + k_9x_8 - k_{10}x_4x_9 \\
f_5 &= k_{14}x_{12} + k_{15}x_{12} + k_{17}x_{13} + k_{18}x_{13} + k_{35}x_{24} + k_{36}x_{24} + k_{41}x_{27} + k_{42}x_{27} - k_{13}x_{11}x_5 - k_{34}x_{16}x_5 \\
&\quad - k_{40}x_{26}x_5 - k_4x_4x_5 + k_5x_6 + k_6x_6 - k_{16}x_5x_9, \\
f_6 &= k_4x_4x_5 - k_5x_6 - k_6x_6, & f_7 &= k_{18}x_{13} - k_7x_4x_7 + k_8x_8, & f_8 &= k_7x_4x_7 - k_8x_8 - k_9x_8, \\
f_9 &= k_{11}x_{10} + k_{15}x_{12} + k_{17}x_{13} + k_9x_8 - k_{10}x_4x_9 - k_{16}x_5x_9, & f_{10} &= -k_{11}x_{10} - k_{12}x_{10} + k_{10}x_4x_9, \\
f_{11} &= k_{12}x_{10} + k_{14}x_{12} - k_{19}x_{11}x_{14} + k_{20}x_{15} + k_{21}x_{15} - k_{22}x_{11}x_{16} + k_{23}x_{17} + k_{24}x_{17} - k_{13}x_{11}x_5, \\
f_{12} &= -k_{14}x_{12} - k_{15}x_{12} + k_{13}x_{11}x_5, & f_{13} &= -k_{17}x_{13} - k_{18}x_{13} + k_{16}x_5x_9, \\
f_{14} &= -k_{19}x_{11}x_{14} + k_{20}x_{15} + k_{30}x_{21} + k_{36}x_{24}, & f_{15} &= k_{19}x_{11}x_{14} - k_{20}x_{15} - k_{21}x_{15}, \\
f_{16} &= k_{21}x_{15} - k_{22}x_{11}x_{16} + k_{23}x_{17} - k_{28}x_{16}x_{19} + k_{27}x_{20} + k_{29}x_{21} + k_{33}x_{23} + k_{35}x_{24} - k_{34}x_{16}x_5, \\
f_{17} &= k_{22}x_{11}x_{16} - k_{23}x_{17} - k_{24}x_{17}, \\
f_{18} &= k_{24}x_{17} - k_{25}x_{18}x_{19} + k_{26}x_{20} - k_{31}x_{18}x_{22} + k_{32}x_{23} + k_{38}x_{25} + k_{39}x_{25} \\
&\quad - k_{43}x_{18}x_{28} + k_{44}x_{29} + k_{45}x_{29} - k_{37}x_{18}x_4, \\
f_{19} &= -k_{46}x_{19} - k_{28}x_{16}x_{19} - k_{25}x_{18}x_{19} + k_{26}x_{20} + k_{27}x_{20} + k_{29}x_{21} + k_{30}x_{21} + k_{45}x_{29}, \\
f_{20} &= k_{25}x_{18}x_{19} - k_{26}x_{20} - k_{27}x_{20}, & f_{21} &= k_{28}x_{16}x_{19} - k_{29}x_{21} - k_{30}x_{21}, \\
f_{22} &= -k_{31}x_{18}x_{22} + k_{32}x_{23} + k_{33}x_{23}, & f_{23} &= k_{31}x_{18}x_{22} - k_{32}x_{23} - k_{33}x_{23}, \\
f_{24} &= -k_{35}x_{24} - k_{36}x_{24} + k_{34}x_{16}x_5, & f_{25} &= -k_{38}x_{25} - k_{39}x_{25} + k_{37}x_{18}x_4, \\
f_{26} &= k_{39}x_{25} + k_{41}x_{27} - k_{40}x_{26}x_5, & f_{27} &= -k_{41}x_{27} - k_{42}x_{27} + k_{40}x_{26}x_5 \\
f_{28} &= k_{46}x_{19} - k_{43}x_{18}x_{28} + k_{44}x_{29}, & f_{29} &= k_{43}x_{18}x_{28} - k_{44}x_{29} - k_{45}x_{29}.
\end{aligned}$$

After some obvious factorization, the following elements are binomials: $f_2, f_6, f_8, f_{10}, f_{12}, f_{13}, f_{15}, f_{17}, f_{20}, f_{21}, f_{22}, f_{23}, f_{24}, f_{25}, f_{27}, f_{29}$. The system has seven conservation relations, which can be found by linear algebra. According to our strategy to use binomials to simplify the system, we eliminate, if possible, non-binomials using the conservation relations. This is not always possible, as some of the conservation relations stem from duplicate equations like $f_2 = -f_3$. We eliminate $f_3, f_4, f_5, f_8, f_9, f_{18}$, and f_{19} . The remaining non-binomial part consists of $f_1, f_7, f_{11}, f_{14}, f_{16}, f_{26}$, and f_{28} . Dividing by reaction constants, each of the binomials is of the form $x_i = Kx_jx_l$ for some rational expression K involving only reaction constants. Using these in the non-binomials yields

$$\begin{aligned}
f'_1 &= -\frac{k_1k_3x_1x_2}{k_2 + k_3} + \frac{k_4k_6x_4x_5}{k_5 + k_6}, & f'_7 &= -\frac{k_7k_9x_4x_7}{k_8 + k_9} + \frac{k_{16}k_{18}x_5x_9}{k_{17} + k_{18}}, \\
f'_{11} &= -\frac{k_{13}k_{15}x_{11}x_5}{k_{14} + k_{15}} + \frac{k_{10}k_{12}x_4x_9}{k_{11} + k_{12}},
\end{aligned}$$

$$\begin{aligned}
f'_{14} &= -\frac{k_{19}k_{21}x_{11}x_{14}}{k_{20}+k_{21}} + \frac{k_{28}k_{30}x_{16}x_{19}}{k_{29}+k_{30}} + \frac{k_{34}k_{36}x_{16}x_5}{k_{35}+k_{36}}, \\
f'_{16} &= \frac{k_{19}k_{21}x_{11}x_{14}}{k_{20}+k_{21}} - \frac{k_{22}k_{24}x_{11}x_{16}}{k_{23}+k_{24}} - k_{28}x_{16}x_{19} + \frac{k_{28}k_{29}x_{16}x_{19}}{k_{29}+k_{30}} + \frac{k_{25}k_{27}x_{18}x_{19}}{k_{26}+k_{27}} \\
&\quad + \frac{k_{31}k_{33}x_{18}x_{22}}{k_{32}+k_{33}} - k_{34}x_{16}x_5 + \frac{k_{34}k_{35}x_{16}x_5}{k_{35}+k_{36}}, \\
f'_{26} &= \frac{k_{37}k_{39}x_{18}x_4}{k_{38}+k_{39}} - \frac{k_{40}k_{42}x_{26}x_5}{k_{41}+k_{42}}, \quad f'_{28} = k_{46}x_{19} - \frac{k_{43}k_{45}x_{18}x_{28}}{k_{44}+k_{45}}.
\end{aligned}$$

In particular, we find five new binomials f'_1 , f'_7 , f'_{11} , f'_{26} , and f'_{28} . Adding f'_{14} to f'_{16} yields the trinomial

$$f''_{16} = -\frac{k_{22}k_{24}x_{11}x_{16}}{k_{23}+k_{24}} + \frac{k_{25}k_{27}x_{18}x_{19}}{k_{26}+k_{27}} + \frac{k_{31}k_{33}x_{18}x_{22}}{k_{32}+k_{33}}.$$

Consequently, the original system is equivalent to a system consisting of 27 binomials and two trinomials of a relatively simple shape. For comparison we computed the Gröbner basis in MACAULAY2 with rational functions in the reaction rates as coefficients. Although the computation finished in just 18 minutes, the result is practically unusable. The Gröbner basis consists of 169 elements each of it with huge rational functions as coefficients. The structure that we observed above is completely lost.

The lesson learned from Example 4.4 is that term replacements using binomials are useful in solving a polynomial system, even if the end result is not binomial. Especially in the non-homogeneous case where the notion of minimal generators is absent, computations with the BINOMIALS package [16] in MACAULAY2 [11] can probably only assist, but not automatically do useful reductions. For example, a natural general choice would be to replace higher degree monomials by lower degree ones, but this would not directly reveal binomiality in Example 4.3.

Finally, we summarize a possible strategy to deal with inhomogeneous ideals. Example 4.1, for instance, is solved already by item 1, but also by item 3.

Recipe 4.5.

- 1) Try linear algebra and Proposition 2.5.
- 2) Homogenize the given ideal and run Algorithm 3.3. If the algorithm returns binomials, then by Proposition 4.2 the original (dehomogenized) ideal is binomial. The homogenization should be carried out after linear algebra reductions to possibly detect homogeneity already at an earlier stage (compare Example 2.8).
- 3) If Algorithm 3.3 returns a negative answer, dehomogenize and use known binomials for term replacements (as in Example 4.4). Potentially homogenize again with an enlarged generating set.
- 4) Compute a reduced Gröbner basis.

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